# When finite-size corrections vanish: The $S = 1/2$ XXZ model and the Razumov-Stroganov state

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We study the one-dimensional $S = 1/2$ XXZ model on a finite lattice at zero temperature, varying the exchange anisotropy $\Delta$ and the number of sites $N$ of the lattice. Special emphasis is given to the model with $\Delta = 1/2$ and $N$ odd, whose ground state, the so-called Razumov-Stroganov state, has a peculiar structure and no finite-size corrections to the energy per site. We find that such model corresponds to a special point on the $\Delta$-axis which separates the region where adding spin-pairs increases the energy per site from that where the longer the chain the lower the energy. Entanglement properties do not hold surprises for $\Delta = 1/2$ and $N$ odd. Finite-size corrections to the energy per site non trivially vanish also in the ferromagnetic $\Delta \to -1^+$ isotropic limit, which is consequently addressed; in this case, peculiar features of some entanglement properties, due to the finite length of the chain and related with the change in the symmetry of the Hamiltonian, are evidenced and discussed. In both the above models the absence of finite-size corrections to the energy per site is related to a peculiar structure of the ground state, which has permitted us to provide new exact analytic expressions for some correlation functions.

## I. INTRODUCTION

Low dimensional magnetic systems have been acknowledged as intriguing physical systems for decades and still attract much interest, both from the theoretical and the experimental point of view. Many reasons justify such interest, and one more has been recently added, namely the possibility to use $S = 1/2$ spin models as tools for studying problems related to quantum information theory and quantum computation [1, 2, 3]. Amongst one-dimensional systems, a preminent role is played by the Heisenberg Hamiltonian

$$\mathcal{H} = \sum_i \left( J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right) , \qquad (1)$$

where $i$ runs over the sites of a chain, and $S_i$ are angular momentum operators satisfying $[S_i^\alpha, S_j^\beta] = i\delta_{ij}\varepsilon^{\alpha\beta\gamma} S_i^\gamma$ $(\alpha, \beta, \gamma = x, y, z)$. Models described by the Hamiltonian (1) constitute a class which is characterized, even at zero temperature, by the possible occurrence of peculiar phenomena, such as quantum phase transitions [4], saturation [5, 6, 7], or factorization [8, 9]. Whether a specific model displays one such phenomenon depends on the details of the exchange interaction and, in case, on the value of an external magnetic field. The values of the exchange parameters $J_x$, $J_y$ and $J_z$ define each model, which in fact may get its name after such values.

In this paper we will refer to the $S = 1/2$ XXZ chain with a finite number of sites $N$ and periodic boundary conditions, whose Hamiltonian can be written in the dimensionless form

$$\mathcal{H} = \sum_{i=1}^{N} \left[ -(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \Delta \sigma_i^z \sigma_{i+1}^z \right] , \qquad (2)$$

where $\sigma_i^\alpha$ are the Pauli matrices for the spin sitting at site $i$. The above expression is obtained from Eq. (1) by setting $J_x = J_y = -4$ and $J_z = 4\Delta$. The choice of the minus sign in front of the exchange interaction on the $xy$-plane implies no loss of generality in the thermodynamic limit, due to the possibility of changing such sign at will via a unitary transformation. However, when finite chains are considered, special care is due to this aspect, as explained in Section II.

The behaviour of the model depends on the value of the anisotropy parameter: isotropic ferro- ($\Delta = -1$) or antiferromagnetic ($\Delta = 1$); Ising-like ($|\Delta| > 1$); critical ($|\Delta| < 1$). Within each interval, the actual value of $\Delta$ is not of particular interest, at least as far as the general phenomenology is concerned. However, in the case of the XXZ model Eq. (2) there exists an exception to this statement: In fact, for $\Delta = 1/2$, periodic boundary conditions, and a finite and odd number of sites, the ground state of the model, often referred to as the Razumov-Stroganov state, shows very peculiar features [10, 11, 12] which still stand as an unintelligible occurrence. Such features do not fall within the framework of quantum phase transitions, as the model lies well inside the $|\Delta| < 1$ region of the XXZ Hamiltonian; moreover, the matter is relevant only as far as the number of sites of the chain is finite, so that the difference between odd and even number of sites stays meaningful.

The Razumov-Stroganov state has been studied by several authors (see for example Refs. [13, 14, 15, 16]), with different approaches and in many different frameworks, but somehow neglecting the fact that the corresponding model is not isolated in the phase diagram of the XXZ model.

In this paper, we tackle the problem from a different point of view: Given the fact that a very peculiar ground

state occurs only for $\Delta = 1/2$ and odd number of sites, we develop a comparative analysis of the behaviour of other XXZ models, i.e. models defined by Eq. (2) with $\Delta \neq 1/2$, and $N$ both even and odd, looking for clues about what in fact makes the model whose ground state is the Razumov-Stroganov state so special. From a physical perspective, one of the most interesting feature of the Razumov-Stroganov state is the absence of finite-size corrections to its energy per site. This property is shared by the fully separable ground state of the finite-length ferromagnetic isotropic ($\Delta = -1$) chain and also by the ground state of the $\Delta \to -1^+$ limit, whose structure is however not as trivial, and deserves special attention.

In the above framework, we have analyzed the effects of the finite length of the chain on the energy, the correlation functions, and some entanglement properties. The analysis presented is based on exact (i.e. available with infinite precision) results as far as the Razumov-Stroganov state and the ground state of the $\Delta \to -1^+$ model are concerned, and on numerical data in all the other cases. Numerical diagonalization techniques underlie all our outcomes.

The structure of the paper is as follows: In Section II we introduce the Razumov-Stroganov state and briefly recall its structure and properties. Some new exact results for the two-point correlation functions of the corresponding chain ($\Delta = 1/2$ and $N$ odd) are also presented. In Section III we consider the energy and the correlation functions at $T = 0$ of several XXZ models, with $|\Delta| < 1$ and $N$ both even and odd, focusing our attention upon finite-size corrections. In Section IV the same type of analysis is proposed for some entanglement properties at $T = 0$. Conclusions are drawn in Section V.

Some exact analytic expressions for the correlation functions of the $\Delta = 1/2$ and the $\Delta \to -1^+$ models are presented in the two Appendices.

## II. SPECIFICITY OF THE VALUE $\Delta = 1/2$

Let us consider the XXZ Hamiltonian (2) on a finite chain with periodic boundary conditions and $N$ odd, at the particular value $\Delta = 1/2$:

$$\mathcal{H} = \sum_{i=1}^{N} \left[ -(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \frac{1}{2} \sigma_i^z \sigma_{i+1}^z \right] , \\ \vec{\sigma}_{N+1} = \vec{\sigma}_1 ; \qquad N \text{ odd} . \tag{3}$$

It is worth noticing that, due to the specific conditions on the lattice, the negative sign of the transverse coupling cannot be reversed at will: Indeed, the rotation of $\pi$ around the $z$-axis of all the spins sitting at every other site can be safely performed only in the case of $N$ even, or in the thermodynamic limit.

The ground state of the above Hamiltonian is doubly degenerate for any $N$ finite and odd, and the two degenerate ground states are eigenstates of $\sum_{i=1}^N S_i^z$, with eigenvalue $S_{tot}^z = \pm 1/2$. The two ground states are obtained from each other reversing the component along the quantization axis of each spin, and their structure is that of the so-called Razumov-Stroganov state. In the following we shall always refer to the $S_{tot}^z = +1/2$ case.

The Razumov-Stroganov state shows several intriguing properties [10, 11, 12]: *i)* its energy per site reads exactly $E/N = -\frac{3}{2}$, with no finite-size corrections; *ii)* the coefficients of the ground state on the *standard* basis (i.e. the basis where all operators $\sigma_i^z$, $i = 1, \dots N$ are diagonal), are integer multiples of the smallest one; *iii)* some of these integer numbers have a non trivial combinatorial interpretation.

A complete understanding of these features is still lacking. It is worth recalling that the XXZ chain with $\Delta = 1/2$ is known to have a similarly special ground state in two other cases: *a*) twisted boundary conditions and $N$ even [10, 17]; *b*) open boundary conditions for whatever $N$, even or odd [10, 18].

The fact that, when suitably normalized, the coefficients defining the ground state of Eq. (3) on the standard basis are all integers (see point *ii)* above) allows for their *exact* numerical evaluation [19, 20], for $N$ not too large, limited only by computing capabilities. Indeed we have computed numerically these integer-valued coefficients with infinite precision, on a standard desktop computer, for system sizes up to $N = 25$. From the exact knowledge of the ground state the correlation functions are readily determined and, as in the present case they necessarily assume rational values, we have computed them with infinite precision, again for chain lengths up to $N = 25$. We report in Appendix A, for illustrative purposes, some of our results for the second neighbour longitudinal two-point correlation function $\langle \sigma_i^z \sigma_{i+2}^z \rangle_N$. Here and below $\langle \dots \rangle_N$ denotes the expectation value over the ground state of a chain of $N$ spins. Further results are available upon request [19].

It appears that the knowledge of the exact values of such correlation functions for a finite set of values of $N$, together with the fact that these are rational numbers, allows to determine their analytic expressions as functions of $N$ (obviously, only valid for odd $N$). This is a rather exceptional situation for an interacting critical system. In particular, from the infinite-precision data mentioned above, and the exact thermodynamic-limit values computed in Refs. [21] and [22], we have been able to work out exact analytic expressions for the $r^{\text{th}}$-neighbour longitudinal and transverse two-point correlation functions, for $r = 1, 2, 3, 4, 5$, and arbitrary $N$. The expressions for $r = 1$ coincide with those computed by means of purely analytic methods in Ref. [11]

$$\langle \sigma_i^+ \sigma_{i+1}^- \rangle_N = \frac{5}{16} + \frac{3}{16N^2} , \quad \langle \sigma_i^z \sigma_{i+1}^z \rangle_N = -\frac{1}{2} + \frac{3}{2N^2} , \tag{4}$$

while those for $r = 2, 3, 4, 5$ were previously unknown. We report them in Appendix A.

Let us briefly illustrate the method used in deriving such expressions, taking as an example the case

of the second-neighbour longitudinal two-point correlation function $\langle\sigma_i^z\sigma_{i+2}^z\rangle_N$, whose exact values for $N = 3, 5, \ldots, 15$, are reported in Appendix A. Subtracting from such values the corresponding exact value in the thermodynamic limit (in this case, 7/64, see [21]), and factoring into prime numbers the resulting denominators, it is easy to infer for these denominators a behaviour, as a function of $N$, of the form $2^6N^2(N^2-4)$. The corresponding numerators are also expected to behave as a polynomial in $N$, although of lower order, since the fraction as a whole should vanish in the thermodynamic limit. The first four values of $\langle\sigma_i^z\sigma_{i+2}^z\rangle_N$, for $N = 3, 5, 7, 9$, are sufficient to determine the polynomial in the numerator, thus completely fixing the expression of $\langle\sigma_i^z\sigma_{i+2}^z\rangle_N$ for arbitrary $N$, see Eq. (A2). The obtained expression reproduces exactly the available numerical values of $\langle\sigma_i^z\sigma_{i+2}^z\rangle_N$, for $N$ larger than 9. From a strictly mathematical point of view, the results of such procedure can only be conjectural, though strongly supported by the numerical data.

The above procedure can be applied to $r^{\rm th}$-neighbour correlation functions, but the degree of the involved polynomials increases rapidly. For generic values of $r$, the denominators appears to behave as $N^{2[(r+1)/2]}\prod_{i=1}^{[r/2]}(N^2-4i^2)^{r-2i+1}$. When $r = 6$, for example, the denominator is of degree 24 in $N$, and even under the reasonable assumption (supported by all lower-$r$ examples) that the numerator is an even polynomial in $N$, we need 12 data to determine it, and possibly one more to check the result. These data can be taken from the values for $N = 7, 9, \ldots 31$, which however lie beyond our computing capabilities. In this respect it is worthwhile to emphasize that, although the derivation of the results presented above and in Appendix A rely heavily on computer aided evaluations, they are all *exact*.

## III. OTHER MODELS

In this Section we aim at getting some deeper insight into the physical mechanisms possibly related to the peculiar ground state of Hamiltonian (3); in particular, we wish to highlight the specific role played by each of the two conditions defining the model, i.e. $\Delta = 1/2$ and $N$ finite and odd (in the case of periodic boundary conditions); to this purpose we develop a comparative analysis of the behaviour of other XXZ models, i.e. models defined by Eq. (2) with $\Delta \neq 1/2$, for different values of $N$.

We first recall that, despite the most spectacular features being observed for $N$ odd, the model (3) has a precise specificity also in the thermodynamic limit. In fact, as demonstrated by Baxter in Ref. [23], whenever the exchange parameters of an infinite Heisenberg chain, Eq. (1), satisfy the condition

$$J_xJ_y + J_xJ_z + J_yJ_z = 0 \tag{5}$$

the energy per site $E/N$ of the ground state gets the value

$$\frac{1}{4}(J_x + J_y + J_z)\ ; \tag{6}$$

in the case of the XXZ model (2), this may only occur for $\Delta = 1/2$, a condition which therefore defines a somehow *special* point, though by no means related with quantum critical transitions, nor with possible factorization or saturation of the ground state.

In Section II we have seen that one of the most intriguing peculiarities of the model Eq. (3) is that finite-size corrections do not enter the energy expression, which necessarily implies $\langle\mathcal{H}\rangle_N/N = -3/2$, given that condition (5) is fulfilled. Due to translation invariance, and given that $\mathcal{H} = \sum_i \mathcal{H}_{i,i+1}$, the absence of finite-size corrections is a property of the local energy, by this meaning that the expectation value of the nearest-neighbour interaction is not affected by the possible addition of no matter how many spin-pairs (though adding one single spin would drastically change the whole picture, bridging the model to the essentially different case of $N$ even); the above feature is seen to follow from the exact cancellation of the $N$-dependent terms in the nearest-neighbour correlation functions, when combined as necessary: In fact, by Eqs. (4), it is

$$\begin{aligned}\langle\mathcal{H}_{i,i+1}\rangle_N &= -4\langle\sigma_i^+\sigma_{i+1}^-\rangle_N + \frac{1}{2}\langle\sigma_i^z\sigma_{i+1}^z\rangle_N \\ &= -\frac{5}{4} - \frac{3}{4N^2} - \frac{1}{4} + \frac{3}{4N^2} = -\frac{3}{2}\ ,\end{aligned} \tag{7}$$

which shows that, despite the correlation functions being affected by finite-size corrections, the interaction energy is not.

Let us now analyze how XXZ models behave for different values of $N$ and $\Delta$. For the sake of clarity, the finite-size corrections relative to any physical observable $\mathcal{O}$ will be hereafter studied in terms of the quantity $\delta_N(\mathcal{O})$ defined by

$$\delta_N(\mathcal{O}) = \langle\mathcal{O}\rangle_N - \lim_{M\to\infty}\langle\mathcal{O}\rangle_M\ . \tag{8}$$

We first consider $\delta_N(\mathcal{H}_{i,i+1})$ which is shown in Fig. 1 for different values of $\Delta$ and as a function of $N$: The qualitative difference between even (upper panel) and odd (lower panel) number of sites is evident: finite-size corrections are negative for all values of $\Delta$ and $N$, except $\Delta \geq 1/2$ and $N$ odd.

In other terms, while in general the energy per site increases with the size of the chain, a special situation occurs for odd $N$ and $1/2 < \Delta < 1$, where adding spin pairs lowers the energy: Within the odd-$N$ sector, Hamiltonian (3) is hence found to correspond to the separating case between these two qualitatively different behaviours of the finite-size corrections in the energy of the ground state. The Insets in Fig. 1 show how $E/N$ varies with $N$ for various anisotropies in the vicinity of the value $\Delta = 1/2$: It is evident that such value is crossed with continuity, both in the odd- and in the even-$N$ sector;

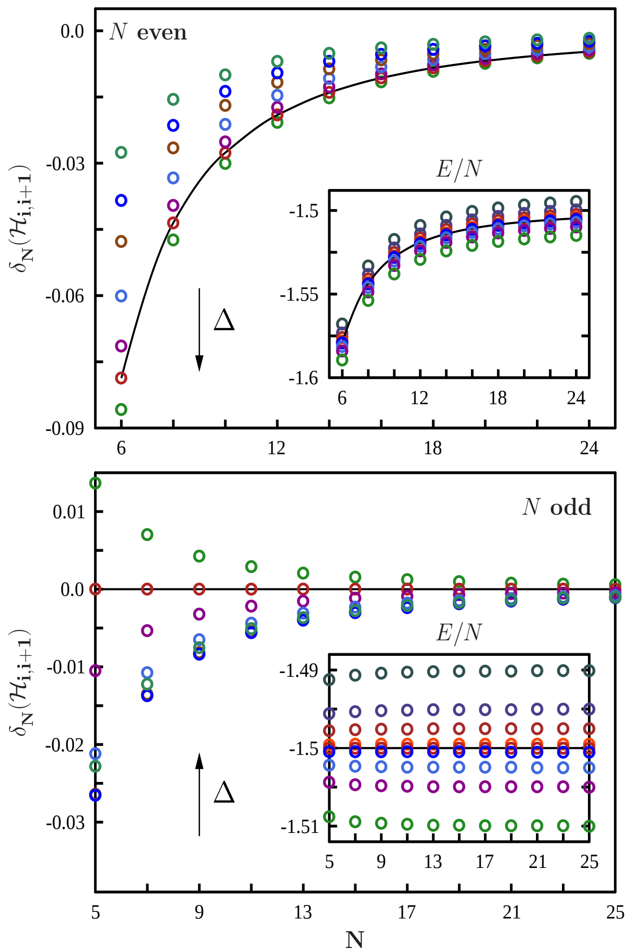


FIG. 1: $\delta_N(\mathcal{H}_{i,i+1})$ versus $N$ for $\Delta = 0.7$, 0.5, 0.3, 0, -0.3, -0.5, -0.7. The full line is a guide for the eyes and connects data for $\Delta = 1/2$. Insets: $E/N$ versus $N$ for $\Delta$= 0.48, 0.49, 0.495, 0.499, 0.50, 0.501, 0.505, 0.51, 0.52. The anisotropy parameter $\Delta$ grows as indicated by the arrows. Upper panel: $N$ even; lower panel: $N$ odd.

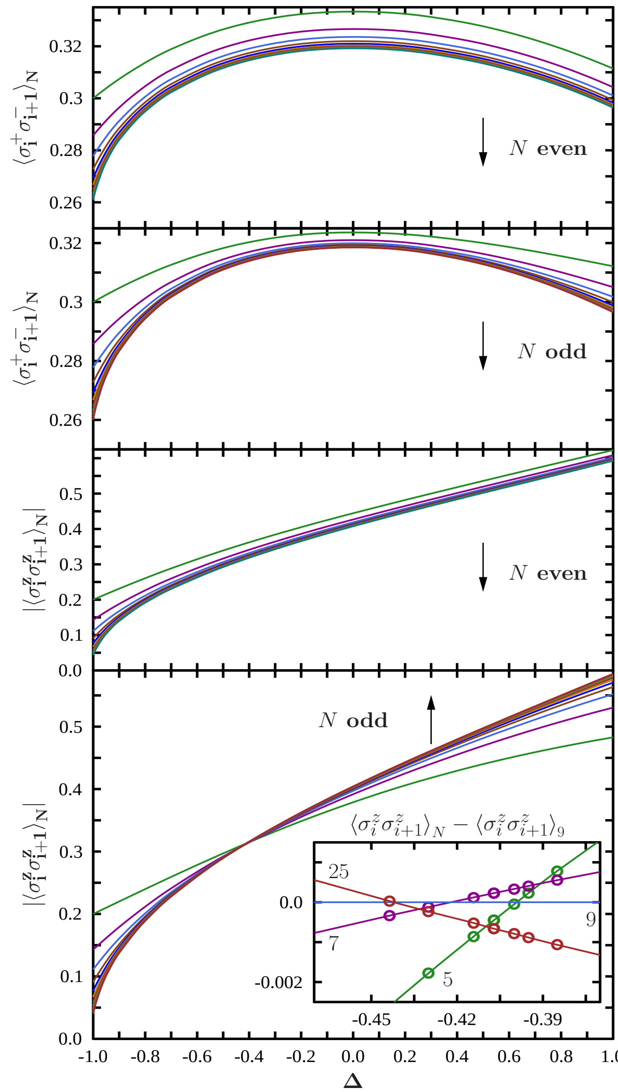


FIG. 2: Nearest-neighbour correlation functions $\langle\sigma_i^+\sigma_{i+1}^-\rangle_N$, and $|\langle\sigma_i^z\sigma_{i+1}^z\rangle_N|$ versus $\Delta$ for different values of $N$ odd and even. $N$ grows as indicated by the arrows, from 5 to 25. The Inset shows the difference $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N - \langle\sigma_i^z\sigma_{i+1}^z\rangle_9$ as a function of $\Delta$, for $N$=5, 7, 9, and 25.

this particularly means, in the former case, that finite-size corrections smoothly vanish for $\Delta \to 1/2$. A simple perturbative analysis for very small $\epsilon = \Delta - 1/2$ yields

$$\frac{E}{N} \simeq -\frac{3+\epsilon}{2} + \frac{3\epsilon}{2N^2} \ , \qquad (9)$$

in complete agreement with the above scenario.

It is to be noticed that the existence of a unique value of $\Delta$, where $\delta_N(\mathcal{H}_{i,i+1})$ changes its sign *for all* values of $N$ odd, is definitely not granted, as shown below in the case of the nearest-neighbour correlation functions along the $z$-direction.

Before considering the correlation functions, we remind that our results are obtained via the numerical diagonalization of the Hamiltonian, so that not only some physical observables, but all the coefficients of the ground state on the standard basis are available, for $N$ both even and odd. This allows us to notice the following general features of the ground state of the XXZ model with $|\Delta| < 1$: *i*) all the elements of the standard basis belonging to the sector with $S^z_{tot} = 1/2$ for $N$ odd, or $S^z_{tot} = 0$ for $N$ even, enter the decomposition of the ground state; *ii*) the coefficients on the standard basis grow with the number of antiparallel adjacent spin pairs featuring the corresponding element; *iii*) keeping the minimum coefficient fixed to unity, all the other coefficients grow with $\Delta$; *iv*) the coefficients are all equal in the $\Delta \to -1^+$ limit.

We further underline, due to its relevance for the following discussion, that the nearest-neighbour correlation functions along the $z$-direction are negative not

only for $\Delta > 0$, as expected, but also for $-1 < \Delta \leq 0$. Indeed, although the exchange interaction in the $z$-direction is ferromagnetic, configurations where adjacent spins have opposite components along the $z$-axis are energetically favoured by the predominant exchange interaction in the $xy$-plane, which is $(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) = 2(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+)$. For the sake of clarity, in the lowest panels of Fig. 2 we plot the absolute values of $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N$.

We now focus upon the finite-size corrections to the quantities $\langle\sigma_i^+\sigma_{i+1}^-\rangle_N$ and $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N$: From Fig. 2 it is clear that $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N$ for odd $N$ behaves in a peculiar way: in fact, while $\delta_N(\sigma_i^+\sigma_{i+1}^-)$ is always positive (the longer the chain the less correlated adjacent spins are on the $xy$-plane), we find that for any odd $N$ it exists a value of $\Delta$ where $\delta_N(\sigma_i^z\sigma_{i+1}^z)$ changes its sign, so that, as far as the anisotropy is larger than such value, adjacent spins get more and more correlated along the $z$-direction as the length of the chain grows, while the opposite occurs otherwise. It is to be noticed that, at variance with the case of $\delta_N(\mathcal{H}_{i,i+1})$, the value of $\Delta$ where $\delta_N(\sigma_i^z\sigma_{i+1}^z)$ vanishes does depend on $N$. This numerical observation is made evident by plotting the difference $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N - \langle\sigma_i^z\sigma_{i+1}^z\rangle_{N'}$ for different values of $N$ and fixed $N'$: should finite-size corrections vanish at a precise value of $\Delta$ indipendently on $N$, all the lines in the Inset of Fig. 2 (where we have chosen $N' = 9$) would cross at the same point, which is seen not to be the case.

Let us now discuss the above results. We have found that nearest-neighbour correlation functions along the $z$-direction in the $S = 1/2$ XXZ model with $\Delta > -1$ are always negative due to prevailing role of the exchange interaction on the $xy$-plane, which evidently favours configurations with antiparallel adjacent spins. On the other hand, the necessary occurrence, in the case of $N$ odd, of at least one pair of adjacent spins with the same component along the $z$-direction, locally frustrates this propensity to antiparallelism. As such constraint concerns just one spin pair, no matter the length of the chain, it may only affect finite-size corrections, and its relevance is smeared out as $N$ increases. This mechanism of local frustration is responsible for the anomalous behaviour of finite-size corrections to $\langle\sigma_i^z\sigma_{i+1}^z\rangle_N$ for $N$ odd, and specifically for the change of sign of $\delta_N(\sigma_i^z\sigma_{i+1}^z)$, which ultimately makes it possible for $\delta_N(\mathcal{H}_{i,i+1}) = -4\delta_N(\sigma_i^+\sigma_{i+1}^-) + \Delta\delta_N(\sigma_i^z\sigma_{i+1}^z)$ to vanish at $\Delta = 1/2$, and stay positive for $\Delta > 1/2$. The model whose ground state has the specific structure predicted by Razumov and Stroganov is thus found to be a special point in the finite-$N$ XXZ phase-diagram, as it separates the region where adding spin pairs increases the energy per site from that where the longer the chain the lower the energy per site.

From this point of view, the XXZ model in the $\Delta \to -1^+$ limit is similarly special (for a precise definition of such model, see Appendix B). Indeed, its ground state has a peculiar structure: It is a superposition with identical coefficients of all the elements of the standard basis within the $S_{tot}^z = 1/2$ ($S_{tot}^z = 0$) sector, for $N$ odd (even). This allows, as shown in Appendix B, for the exact evaluation of the correlation functions. In particular, similarly to Eq. (7), one find, for example for $N$ odd,

$$\begin{aligned}\langle\mathcal{H}_{i,i+1}\rangle_N &= -4\langle\sigma_i^+\sigma_{i+1}^-\rangle_N - \langle\sigma_i^z\sigma_{i+1}^z\rangle_N = \\ &= -1 - \frac{1}{N} + \frac{1}{N} = -1 \ , \end{aligned} \tag{10}$$

and analogously for $N$ even. We thus see that finite-size corrections to the energy per site (but not to other physical quantities) do vanish for this model as well.

We notice that there exists another class of models whose expression for the energy per site is given by Eq. (6), namely any antiferromagnetic XYZ Heisenberg system on a bipartite lattice with periodic boundary conditions, in the presence of a uniform magnetic field whose value fulfills the condition given by Kurman et al. in Ref. [8]. When such condition is fullfilled, the ground state factorizes, meaning that it gets the unexpected classical-like structure of a tensor product of single-spin states. This phenomenon has recently attracted much attention, due to its relevance as far as the entanglement properties are concerned [9, 24, 25, 26]. In this respect, one should notice that while the absence of finite-size corrections in the models studied by Kurmann et al., as well as in the $\Delta = -1$ ferromagnetic isotropic model, directly follows from the factorized structure of the ground state, thus characterizing the expectation value of whatever physical observable, in the Razumov-Stroganov state, as well as in the $\Delta \to -1^+$ ground state, finite-size corrections vanish only in the energy per site, following a precise cancellation in the expectation value of the Hamiltonian.

## IV. ENTANGLEMENT PROPERTIES

The investigation of entanglement properties has revealed a powerful tool in studying spin models, particularly in unveiling peculiar properties of the ground state [27, 28, 29, 30, 31, 32, 33], as in the case of the XYZ antiferromagnet in the uniform field mentioned above [9]. Several authors have specifically addressed the analysis of the XXZ model in terms of entanglement properties [34, 35, 36, 37, 38, 39], and more recently the case of $\Delta = 1/2$ and $N$ odd has been studied in such context [20]. In this framework, the idea that the peculiar structure of the Razumov-Stroganov state might be related with properties of some entanglement measure is suggestive. We have therefore developed the same type of analysis presented in Section III, for the bipartite entanglement between two $S = 1/2$ spins separated by $r$ lattice spacings, as measured by the concurrence [40, 41, 42]

$$C_{r,N} = 2\max\{0, C'_{r,N}\} \ , \tag{11}$$

where

$$C'_{r,N} = \frac{1}{2}\left|\langle\sigma_i^x\sigma_{i+r}^x\rangle_N\right| - \frac{1}{4}\sqrt{\left(1 + \langle\sigma_i^z\sigma_{i+r}^z\rangle_N\right)^2 - 4\langle\sigma_i^z\rangle_N^2} \ . \tag{12}$$

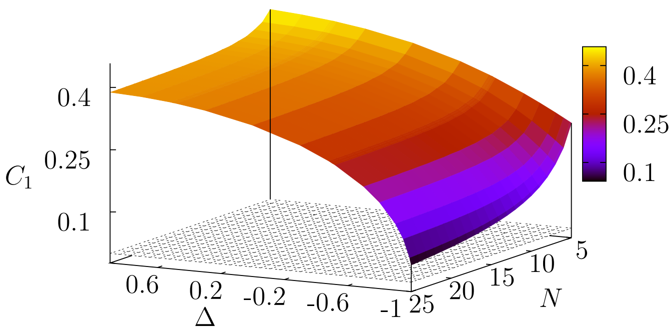


FIG. 3: $C_1$ versus $\Delta$ and $N$

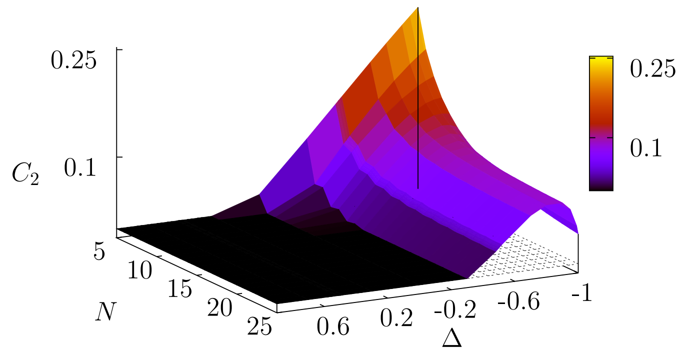


FIG. 4: $C_2$ versus $\Delta$ and $N$

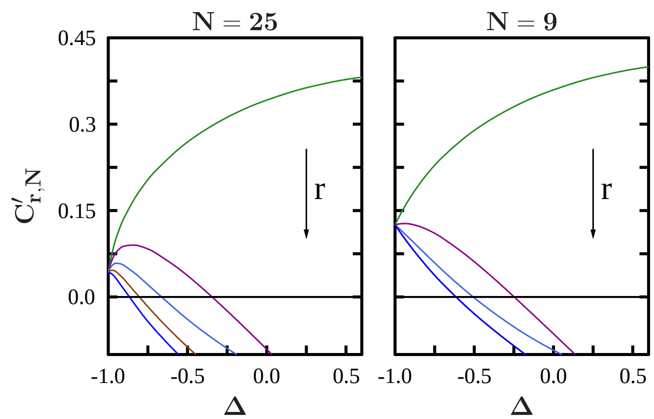


FIG. 5: $C'_{r,N}$ as a function of $\Delta$ for $N = 25$ (left) and $N = 9$ (right) for $r \leq 5$.

We have numerically evaluated $C_{r,N}$ for various $\Delta$, $r$, and $N$. In Figs. 3 and 4 we show $C_{1,N}$ and $C_{2,N}$ versus $N$ and $\Delta$. Apart from very small oscillations between odd and even $N$, essentially due to different finite-size corrections in the correlation functions and to the fact that $\langle\sigma_i^z\rangle_N^2$ in Eq. (12) is positive for $N$ odd and vanishes for $N$ even, no peculiar behaviour is observed. The concurrence between nearest neighbours $C_{1,N}$ is always finite and is larger for larger $\Delta$, i.e. for more marked antiferromagnetic exchange along the $z$-direction (as expected after the analysis presented in Ref. [43, 44]). All pairs of non-adjacent spins are disentangled in the Razumov-Stroganov state, no matter the value of $N$, but this is not a specific feature of the model (3), as already shown by the overall picture presented in Ref. [31]. After all, and despite the particular structure of its ground state, the case $\Delta = 1/2$ and $N$ odd is not found to display peculiar features, at least as far as pairwise entanglement is concerned. The way transverse and longitudinal correlation functions combine in Eq. (12) does not cause any relevant change in the finite-size corrections of the concurrence.

Let us now consider the other point where finite-size corrections to the energy per site vanish, i.e. the ferromagnetic isotropic point $\Delta = -1$. As a matter of fact, the model in the $\Delta \to -1^+$ limit displays features which deserve some comments. In the thermodynamic limit, all the $C_r$ are expected [44] to switch on as $\Delta \to -1^+$, which implies, due to the monogamy inequality [45, 46], that all the concurrences vanish at the ferromagnetic isotropic point $\Delta = -1$, consistently with the fact that the ground state of the XXZ chain with $\Delta \leq -1$ is fully separable. On the other hand, when $N$ is finite (no matter if even or odd), not only all the $C_{r,N}$ switch on as $\Delta \to -1^+$, but they all flow to the same value, as seen in Fig. 5. In particular, from the exact evaluation of the correlation functions reported in Appendix B, one can find that

$$\lim_{\Delta\to-1^+} C_{r,N} = \begin{cases} \frac{N+1}{2N}\left(1-\sqrt{\frac{N-3}{N+1}}\right) & \forall r\ ,\ N \text{ odd}\ ; \\ \frac{1}{N-1} & \forall r\ ,\ N \text{ even}\ . \end{cases} \tag{13}$$

Moreover, when $\Delta < -1$ the result $C_{r,N} = 0$ for all $r$ stays valid also for finite $N$; therefore, and at variance with the thermodynamic limit, a discontinuity of all the concurrences occurs at $\Delta = -1$.

We underline that the one-tangle [45] $\tau = 1 - \sum_\alpha \langle\sigma^\alpha\rangle_N^2$ in the XXZ model with periodic boundary conditions and $|\Delta| < 1$ is different from zero and does not depend on $\Delta$ (being $\tau = 1 - 1/N^2$ for $N$ odd, and $\tau = 1$ for $N$ even), while for $\Delta \leq -1$, $\tau$ vanishes. The observed discontinuity at $\Delta = -1$ (at variance with the one characterizing the concurrence) is not related with the finite size of the system, as it obviously survives in the thermodynamic limit. It is rather connected with the onset of critical behaviour for $|\Delta| < 1$, which implies the vanishing of the magnetizations and a consequently maximal entanglement content.

We understand the mechanism leading to such discontinuities as follows: From our results we observe, as stated in Section III, that the ground state of the XXZ model for $\Delta \to -1^+$ may be written as $P^+ \Pi_i |\varphi\rangle_i$ where $P^+$ is the projector over the Hilbert subspace of the chain corresponding to $S^z_{tot} = 1/2$, and $|\varphi\rangle$ is a single-spin pure state which may be chosen at will, provided it is not one of the two eigenvectors of $\sigma^z$ (so as to ensure the projection does not vanish). The notation indicates that all the spins along the chain are in the same single-spin pure state: In fact, the fully separable state $\Pi_i |\varphi\rangle_i$ is just one of the infinite ground states of the ferromagnetic XXX chain. We therefore see that it is the projection over the $S^z_{tot} = 1/2$ Hilbert subspace which injects entanglement into the fully separable ground state of the ferromagnetic XXX model. We notice that such projection is not a local operation, and it can hence modify the entanglement content of the system. The above reasoning is straightforwardly extended to the $N$ even case, replacing $P^+$ with $P^0$, i.e. with the projector over the $S^z_{tot} = 0$ Hilbert subspace. In other terms, the easy-plane character of the XXZ model with $|\Delta| < 1$, which is embodied in the condition $S^z_{tot} = 1/2$ for $N$ odd, or $S^z_{tot} = 0$ for $N$ even, causes the ground state to develop long-ranged pairwise entanglement as the ferromagnetic isotropic point is approached from above.

Since pairwise entanglement between two spins does not exhaust the possible types of entanglement, and there might be other measures that exhibit a special behaviour near or at $\Delta = 1/2$, we have numerically evaluated the entanglement entropy for a wide range of bipartition of the full chain, and for various $N$ and $\Delta$. In the particular case where the bipartition consists of two blocks of adjacent spins, we find a very good agreement with the theoretical predictions of conformal field theory [47]. Such agreement is observed not only for $\Delta = 1/2$ (as already emphasized in Ref. [20]) but all over the interval $-1 < \Delta < 1$, and $N$ both even and odd. It is worth underlining that such agreement is observed to hold for blocks of at least two spins with great accuracy, even for rather short chains, with $N$ as small as 5.

## V. CONCLUSIONS

Our study of the ground state structure as related with finite-size effects in the one-dimensional $S = 1/2$ XXZ model with periodic boundary conditions in its critical phase ($T = 0$ and $|\Delta| < 1$ ) has highlighted some relevant features; these particularly emerge for $\Delta = 1/2$ and $N$ odd, as well as in the ferromagnetic isotropic limit, $\Delta \to -1^+$ (for $N$ both even and odd). Indeed, these two models share a common property, namely the fact that finite-size corrections to the energy per site vanish, despite being finite as far as other physical quantities are concerned.

In the former case, we have found that the model represents a special point in the $N$-odd sector (where its ground state has the structure of the Razumov-Stroganov state), as it separates the region where adding spin pairs increases the energy per site of the chain, from that where the reverse holds. We think this result, besides giving some further insight into the behaviour of the magnetic XXZ model, could get a specific meaning for the fermionic models whose Hamiltonian is mapped into the $S = 1/2$ XXZ one (see for example Ref. [14]), possibily in terms of a physical mechanism related with a properly defined chemical potential.

In the $\Delta \to -1^+$ limit, the peculiarities of the model do also arise from the very specific (despite not as intriguing as that of the Razumov-Stroganov state) structure of the ground state, which guarantees the exact cancellation of finite-size corrections to the energy per site, for $N$ both even and odd. However, in this case the peculiar ground state structure most relevantly reflects on bipartite entanglement: all the concurrences are finite and get the same value, no matter the distance between the two spins considered. In fact, we have found that there is a region, while approaching the ferromagnetic isotropic point from above, where any two spins along the chain are entangled, given that the finite size of the chain prevents the *monogamy of the entanglement* to force the vanishing of all the concurrences; in such region the entanglement between a selected spin pair can be varied not only by tuning $\Delta$ but also by properly choosing $N$, a possibility which might be relevant in the design of quantum devices.

Finally, we recall that the two above mentioned models, besides sharing a somewhat specific finite-size behaviour, present another rather exceptional peculiarity, namely the possibility of accessing the exact structure of their ground state. Indeed, in both cases, the (suitably normalized) coefficients of the ground state in the standard basis are all integers: This naturally sets the models into the realm of combinatorics, and has permitted us to derive new exact analytic expressions for their correlation functions.


### Acknowledgments

We thank Miguel Ibañez de Berganza, Alessandro Cuccoli, Andrei Pronko and Ruggero Vaia for useful discussions. FC acknowledges partial support from the European Science Foundation program INSTANS, and from MIUR, under the PRIN grant 2007JHLPEZ.


## APPENDIX A: SOME EXACT RESULTS AT $\Delta = 1/2$

We report here the exact values of the second neighbour longitudinal two-point correlation function

$\langle\sigma_i^z\sigma_{i+2}^z\rangle_N$, for $N=3,5,\ldots,15$:

$$\begin{aligned}
\langle\sigma_i^z\sigma_{i+2}^z\rangle_3 &= -\frac{1}{3}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_5 &= \frac{1}{25}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_7 &= \frac{4}{49}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_9 &= \frac{28}{297}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_{11} &= \frac{157}{1573}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_{13} &= \frac{191}{1859}\\
\langle\sigma_i^z\sigma_{i+2}^z\rangle_{15} &= \frac{1732}{16575}
\end{aligned} \tag{A1}$$

Note that all these values are rational numbers. This remarkable property allows for their infinite-precision numerical evaluation, and permits to derive the exact expressions of the correlation functions for arbitrary (odd) values of $N$. We report below our results for the $r^{\text{th}}$-neighbour longitudinal and transverse two-point correlation functions, $r=2,3,4,5$:

$$\langle\sigma_i^z\sigma_{i+2}^z\rangle_N = \frac{7}{2^6} - \frac{3}{2^6}\left(\frac{227+22N^2}{N^2(N^2-4)}\right) \tag{A2}$$

$$\langle\sigma_i^+\sigma_{i+2}^-\rangle_N = \frac{41}{2^8} + \frac{105}{2^8}\left(\frac{1+2N^2}{N^2\,(N^2-4)}\right) \tag{A3}$$

$$\langle\sigma_i^z\sigma_{i+3}^z\rangle_N = -\frac{401}{2^{12}} + \frac{45}{2^{12}}\left(\frac{-2205+5324N^2+26N^4+212N^6}{N^4(N^2-4)^2}\right) \tag{A4}$$

$$\langle\sigma_i^+\sigma_{i+3}^-\rangle_N = \frac{4399}{2^{15}} + \frac{9}{2^{15}}\left(\frac{-11025+1276N^2-7358N^4+4516N^6}{N^4\left(N^2-4\right)^2}\right) \tag{A5}$$

$$\begin{aligned}
\langle\sigma_i^z\sigma_{i+4}^z\rangle_N = \frac{184453}{2^{22}} - \frac{3}{2^{22}N^4\left(N^2-4\right)^3\left(N^2-16\right)}\Big(&16094658825-4071808726N^2\\
&+1675416103N^4-269157300N^6+41497687N^8+2281766N^{10}\Big)
\end{aligned} \tag{A6}$$

$$\begin{aligned}
\langle\sigma_i^+\sigma_{i+4}^-\rangle_N = \frac{1751531}{2^{24}} + \frac{3}{2^{24}N^4\left(N^2-4\right)^3\left(N^2-16\right)}\Big(&4695690825+2413434266N^2\\
&-276248393N^4+556663980N^6-134362697N^8+10926614N^{10}\Big)
\end{aligned} \tag{A7}$$

$$\begin{aligned}
\langle\sigma_i^z\sigma_{i+5}^z\rangle_N = -\frac{95214949}{2^{31}} + \frac{3}{2^{31}N^6\left(N^2-4\right)^4\left(N^2-16\right)^2}\Big(&3019990307709375-1994398549102575N^2\\
+22018044125468N^4-149133792747084N^6&+28928020131522N^8-4476210910162N^{10}\\
&+693645483372N^{12}-43191843804N^{14}+2051652263N^{16}\Big)
\end{aligned} \tag{A8}$$

$$\begin{aligned}
\langle\sigma_i^+\sigma_{i+5}^-\rangle_N = \frac{3213760345}{2^{35}} + \frac{3}{2^{35}N^6\left(N^2-4\right)^4\left(N^2-16\right)^2}\Big(&4227986430793125-565146993503925N^2\\
-383849970492812N^4-183487079646084N^6&+70690548132342N^8-35899621486502N^{10}\\
&+8073828981732N^{12}-796229443764N^{14}+28577677213N^{16}\Big)
\end{aligned} \tag{A9}$$

## APPENDIX B: THE $\Delta \to -1^+$ MODEL

We provide here some analytic results on the XXZ chain of length $N$, in the $\Delta\to -1^+$ limit. It is worth emphasizing that, by construction, this model differs from the isotropic $\Delta=-1$ ferromagnet. It is defined as a limit

from the critical region, and its ground state, together with the expectation value of all physical quantities, is also to be intended as the result of this limit. In particular, the model is critical, with $S^z_{tot} = 1/2$ for $N$ odd, and $S^z_{tot} = 0$ for $N$ even. Setting $\Delta = -1 + \epsilon$, there obviously are finite corrections to all the exact expressions we provide below, but they all vanish as $\epsilon \to 0$.

It is easily seen, from analytic considerations, and numerical experiments, that the ground state of the XXZ chain in the $\Delta \to -1^+$ limit is a superposition with identical coefficients (which we set to unity) of all the elements of the standard basis corresponding to $S^z_{tot} = 1/2$ for $N = 2n+1$ (odd), and to $S^z_{tot} = 0$ for $N = 2n$ (even). Such elements are herafter indicated by $|e_l\rangle$. Their number is $\binom{N}{n}$; the norm of the state consequently reads $\mathcal{N} = \sqrt{\binom{N}{n}}$. Due to the peculiar structure of the ground state, the evaluation of correlation functions reduces to a simple combinatorial enumeration, as shown below.

Let us consider the correlation functions on the $xy$-plane: it is $\langle\sigma^+_i\sigma^-_j\rangle_N = \mathcal{N}^{-2}\sum_{lm}\langle e_l|\sigma^+_i\sigma^-_j|e_m\rangle$, and the elements $|e_m\rangle$ that do contribute to the double sum are just those with $\sigma^z_i|e_m\rangle = -|e_m\rangle$, and $\sigma^z_j|e_m\rangle = |e_m\rangle$; each of them will contribute exactly 1 and their number is $\binom{N-2}{n-1}$, so that

$$\langle\sigma^+_i\sigma^-_j\rangle_N = \frac{N+1}{4N}, \qquad N \text{ odd}, \tag{B1}$$

$$\langle\sigma^+_i\sigma^-_j\rangle_N = \frac{N}{4(N-1)}, \qquad N \text{ even}, \tag{B2}$$

no matter the distance between site $i$ and $j$.

As for the correlation functions along the $z$-axis, it is $\langle\sigma^z_i\sigma^z_j\rangle = \mathcal{N}^{-2}\sum_{lm}\langle e_l|\sigma^z_i\sigma^z_j|e_m\rangle$, and each term in the sum is easily seen to contributes with $\pm\delta_{lm}$. The various terms can be collected, according to the orientation of the $i^{\rm th}$ and $j^{\rm th}$ spins in each $|e_m\rangle$, into four groups, so as to obtain

$$\begin{aligned}\langle\sigma^z_i\sigma^z_j\rangle_N &= \mathcal{N}^{-2}\left[\binom{N-2}{n} - \binom{N-2}{n-1} - \binom{N-2}{n-1} + \binom{N-2}{n-2}\right]\\ &= \frac{(N-2n)^2 - N}{N(N-1)},\end{aligned} \tag{B3}$$

and hence

$$\langle\sigma^z_i\sigma^z_j\rangle_N = -\frac{1}{N}, \qquad N \text{ odd}, \tag{B4}$$

$$\langle\sigma^z_i\sigma^z_j\rangle_N = -\frac{1}{N-1}, \qquad N \text{ even}, \tag{B5}$$

no matter the distance between site $i$ and $j$.

The fact that two-point correlation functions do not depend on the distance is a direct consequence of the particular structure of the ground state, whose non vanishing coefficients on the standard basis are all identical. It is worth mentioning that each of these correlation functions assumes the same value on the chain of length $2n-1$ and $2n$. Finally, notice that these correlation functions have different values with respect to the $\Delta = -1$ isotropic ferromagnetic model. The consequent discontinuity vanishes in the thermodynamic limit.


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